

LifeWatch Italy Annual Conference  
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*in collaboration with the Secretariat General of the Presidency of the Republic*

# Opportunities and challenges of Virtual Research Environments for biodiversity study

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# VREs in biodiversity domains

VREs have the potential to benefit research in all disciplines at all stages of research?



# Permeability of the biodiversity researchers community to VRE innovations

- The permeability level of ICT innovations is generally low biodiversity domain
- Few researchers are aware of the existence of VRE concept
- Many ecologists, zoologists, botanists are field researchers. Sometime they are intimidated also by "normal" computer and are frustated by using complex informatic tools
- Researchers want to use tools that has been proved to work (validated by publications)

# Barriers to the use of VREs

- “...the majority of these systems (VREs) are not yet fully integrated into standard practices, tools and research protocols used by real life communities of practice.”
- “This reluctance to migrate from traditional and consolidated research practices and facilities to the innovative ones promoted by VREs is among the most difficult barriers affecting the entire VRE domain.”

*Candela et al. (2013). Virtual Research Environments: An Overview and a Research Agenda. Data Science Journal. 12, pp.GRDI75–GRDI81*

technology not reliable:	8
too difficult to use:	14
does not suit our research practice:	11
not enough technical support:	22
not enough institutional support for training etc.:	20
user community too small:	15
security/trust issues:	11
other:	36

*Carusi & Reimer, 2010. . Virtual Research Environment Collaborative Landscape Study. JISC*

# LifeWatch VRE

## Virtual Labs

[Resources & Services](#) / Catalogue of Virtual Labs



### Alien and Invasive Species VRE

The LifeWatch Alien Species Virtual Research Environment (AS-VRE) has been built and equipped in order to developing systems that support the scientist's work for experimental researches on alien species arrival and spread into different types of ecosystems (aquatic and terrestrial). The AS-VRE is an example of the types of scientific studies that researchers on biodiversity and AS could undertake.

Would you like to know more [about](#) the Alien Species VRE, its [services](#), get in contact with its [coordination team](#), access the [training](#) resources, view the related [publications](#) and the [showcases](#)? Visit our dedicated [minisite](#).

[AS-VRE minisite](#) ← Back

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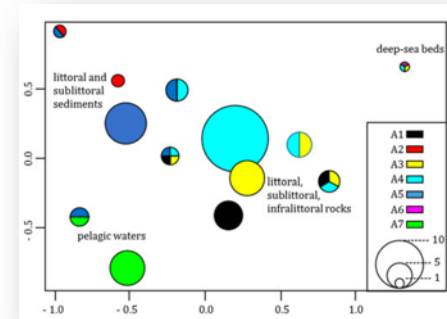
# The Alien Species case study

AQUATIC CONSERVATION: MARINE AND FRESHWATER ECOSYSTEMS

*Aquatic Conserv. Mar. Freshw. Ecosyst.* 26: 392–409 (2016)

Published online 20 February 2015 in Wiley Online Library  
(wileyonlinelibrary.com). DOI: 10.1002/aqc.2550

*Ecosystem vulnerability to alien and invasive species: a case study on marine habitats along the Italian coast*



Aquatic Invasions (2017) Volume 12, Issue 3: 299–309

DOI: <https://doi.org/10.3391/ai.2017.12.3.04>

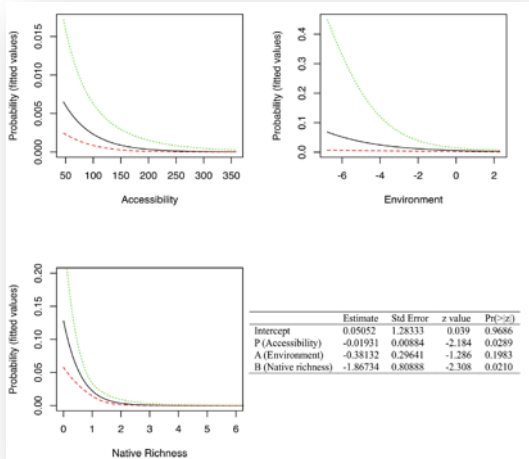
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Open Access

*Special Issue: Invasive Species in Inland Waters*

Research Article

**Alien species in Italian freshwater ecosystems: a macroecological assessment of invasion drivers**



Ecological Indicators 91 (2018) 182–188

Contents lists available at ScienceDirect

Ecological Indicators

journal homepage: [www.elsevier.com/locate/ecolind](http://www.elsevier.com/locate/ecolind)



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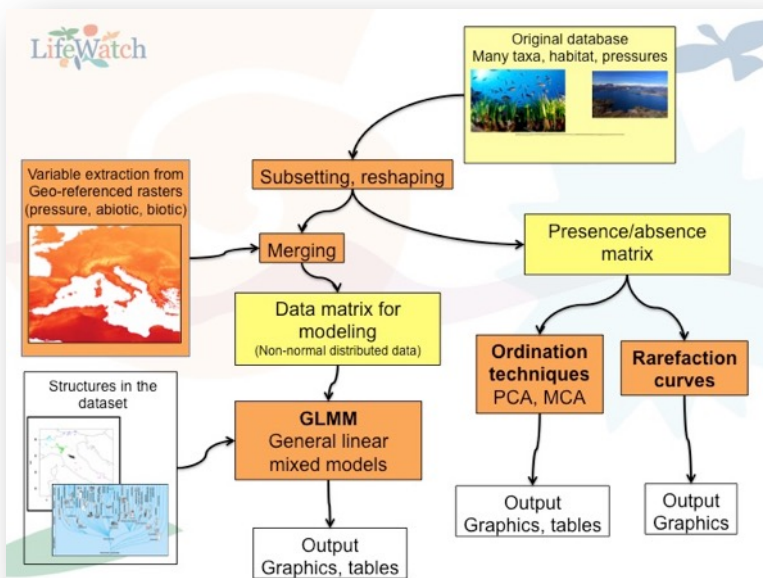
Original Articles

Plant invasions in Italy: An integrative approach using the European LifeWatch infrastructure database



# From statistical workflows to scientific workflows

- Allow users to replicate the workflow
- Allow user to modify the workflow
- Allow user to use their own data, enhancing modularity



```

native_richness<-specnumber(native_table[sapply(native_table, class)!="factor"])
native_richness<-cbind(native_table[sapply(native_table,
class)=="factor"],native_richness)
##merge native+aliene
new_table<-merge(native_richness,alien_richness,all.x=T,all.y=T)
new_table[is.na(new_table)]<-0

# remove unnecessary files
rm("alien_richness")
rm("native_richness")

#####
##
#### Step 2: Generalized Linear Mixed Model (GLMM) fitting usign the lme4 package
####
#####
##

# now we are ready to fit our model. We will use a generalized linear mixed models in
order to take into account the structure of our new dataset. Taxonomic group and
locality are not the focus of our investigation but largely influence our sampling. We
will include these two factor in the random effect.

# First fit full model (a negative binomial family is assumed for richness data)
gfit_Eu_Ri <- glmer.nb(alien_richness ~native_richness+ EunisL1 +(1|
family)+(1|locality), data= new_table)

# automatically calculate best model according to AIC
library(MuMIn)
options(na.action = "na.fail")
ms1<-dredge(gfit_Eu_Ri)
ms1; # the full model has the highest AICc support

# fit the best model according to AIC
mod.fit<-glmer.nb(as.formula(getCall(ms1,1)), data = new_table)

# results
summary(mod.fit) #table.
visreg(mod.fit,trans=exp,nn=101,alpha=1,rug=F,partial=T) #graph

#####
#### Step 3: RAREFACTION CURVES ####
#####


library(vegan)

asfw<-droplevels(subset(freshwater, alien=="1"))
tabella_aspecie<-table(asfw $EunisL1, asfw $scientificname)
rarecurve(tabella_aspecie)
  
```


# Dividi et impera!



iNaturalist occurrences retriever (with Eunis list interaction)



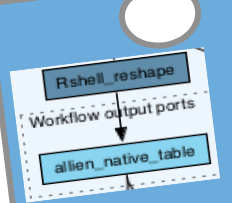
Simple CSV file chooser



LifeWatch Data-portal access

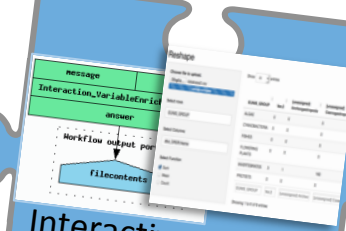


SOS (sensor data) retriever (abiotic vars from LTER Europe)




Rshell\_reshape  
Workflow output ports  
alien\_native\_table

Alien Sp. Workflow reshape (Rshell)

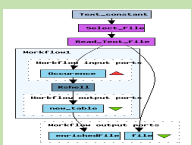


message  
Interaction\_VariableName  
answer  
Workflow output ports  
filecontents

Interactive reshape (shiny interaction)



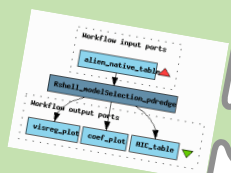
LifeWatch Data-portal REST access



Enrich occurrence with WorldClim (Rshell)

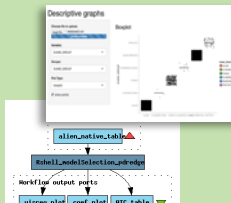


Enrich occurrence with WorldClim (Shiny interaction)



Workflow input ports  
alien\_native\_table  
Rshell\_modelselection\_order  
Workflow output ports  
viewreg\_plot conf\_plot REC\_table

Statistical model selection (Rshell with hard-coded params)



Descriptive graphs  
alien\_native\_table  
Rshell\_modelselection\_order  
Workflow output ports  
viewreg\_plot conf\_plot REC\_table

Statistical model selection (+ choose parameters through descr.stats interaction)



# Enhancing the agent-user interaction

- Progresses: reusable web-application interaction services with **advanced interactivity** and **processing**
- **Taverna aware *Shiny (R)* applications**



## Biotic/Abiotic/Pressure variables extraction

File data  
Select file: occurrence.csv  
Upload complete

Select WorldClim raster layers:

- Bio1
- Bio2
- Bio3
- Bio4
- Bio5

Download Compute  
Use in Taverna

```
"" "longitude", "latitude", "bio2", "bio4"  
"1", -8.76683, 48.56571, 76.3298  
"2", -7.18487, 42.58737, 95.5894  
"3", -7.88494, 42.57335, 96.5171  
"4", -7.88494, 42.57335, 96.5171
```

The interaction service was developed in the [BioVCL project](#)

Some example:

- Enrich species occurrence with abiotic data from WorldClim
- Choices of parameter through *descriptive statistics*
- Dynamically reshape data

## Descriptive graphs

Choose file to upload.  
Browse... biomassa.csv  
Upload complete

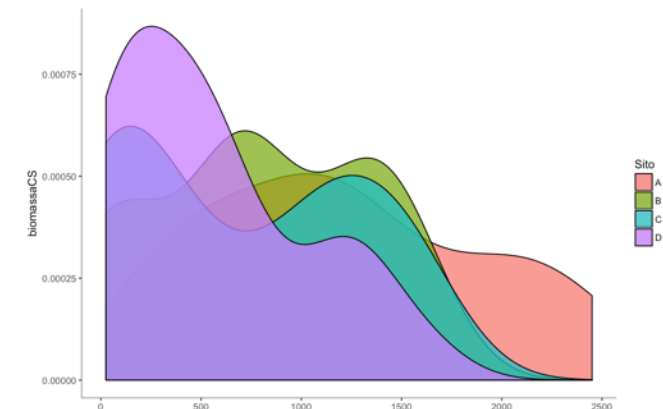
Variable:  
biomassaCS

Groups:  
Site

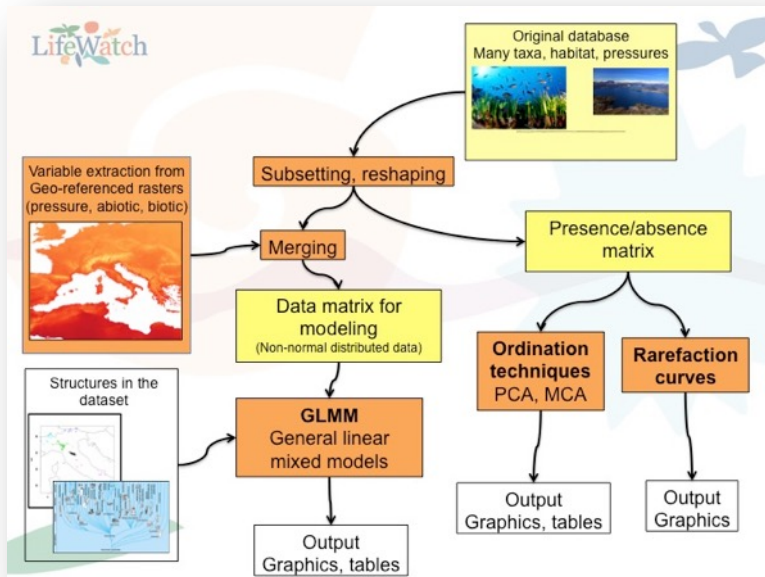
Plot Type:  
density

show points

## Density plot



# From R to Taverna



```
library(shiny)
library(maps)
library(raster)

shinyServer(function(input, output, session) {

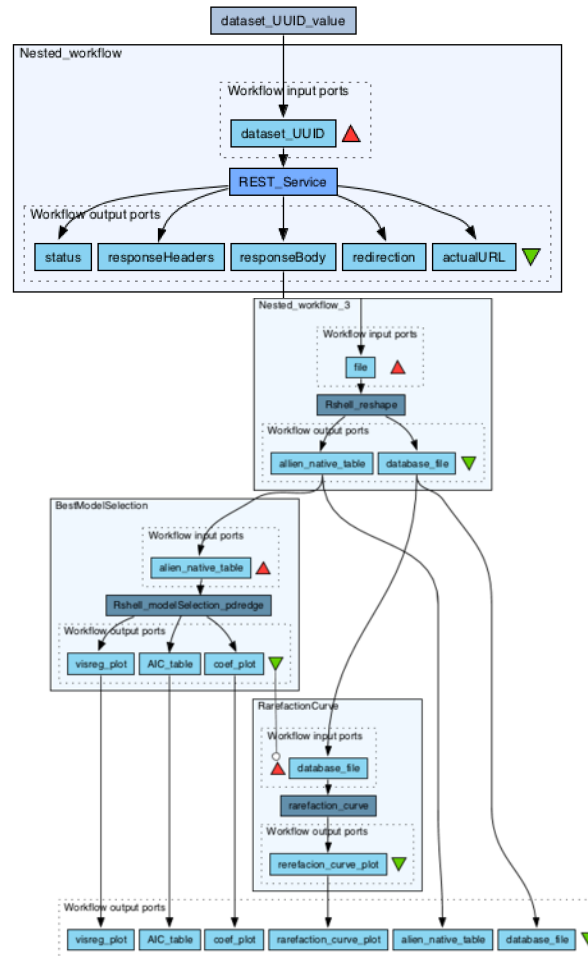
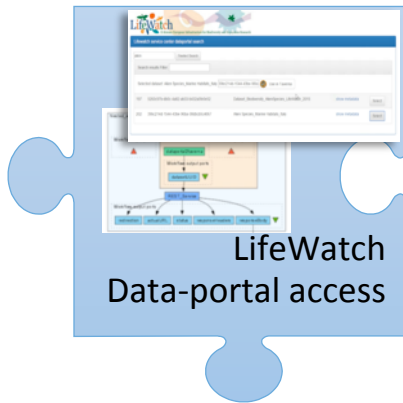
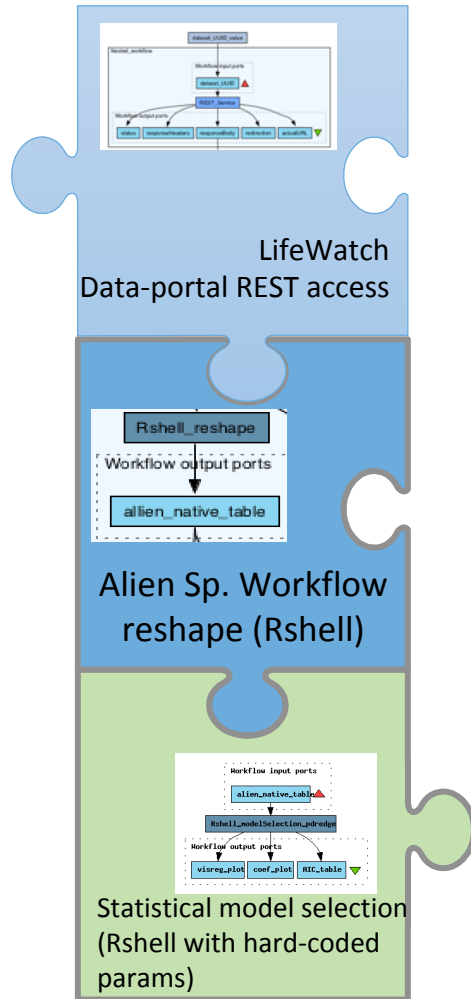
  Data <- reactive({
    inFile<-input$file
    if (is.null(inFile)) {
      return(NULL)
    } else {
      d<-read.csv(inFile$datapath)
    }
  })

  observe({
    data <-Data()
    updateSelectInput(session, "x", choices = names(data))
    updateSelectInput(session, "y", choices = names(data))
  })
})
```

## Taverna service oriented scientific workflow

Implement R scripts via Rshell and Rserve.  
Connect R scripts with other services

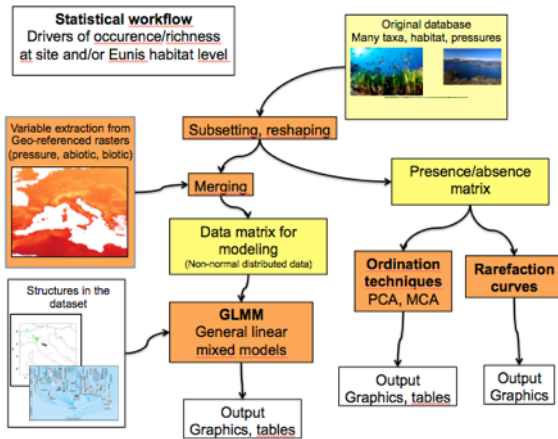
# Re-combination



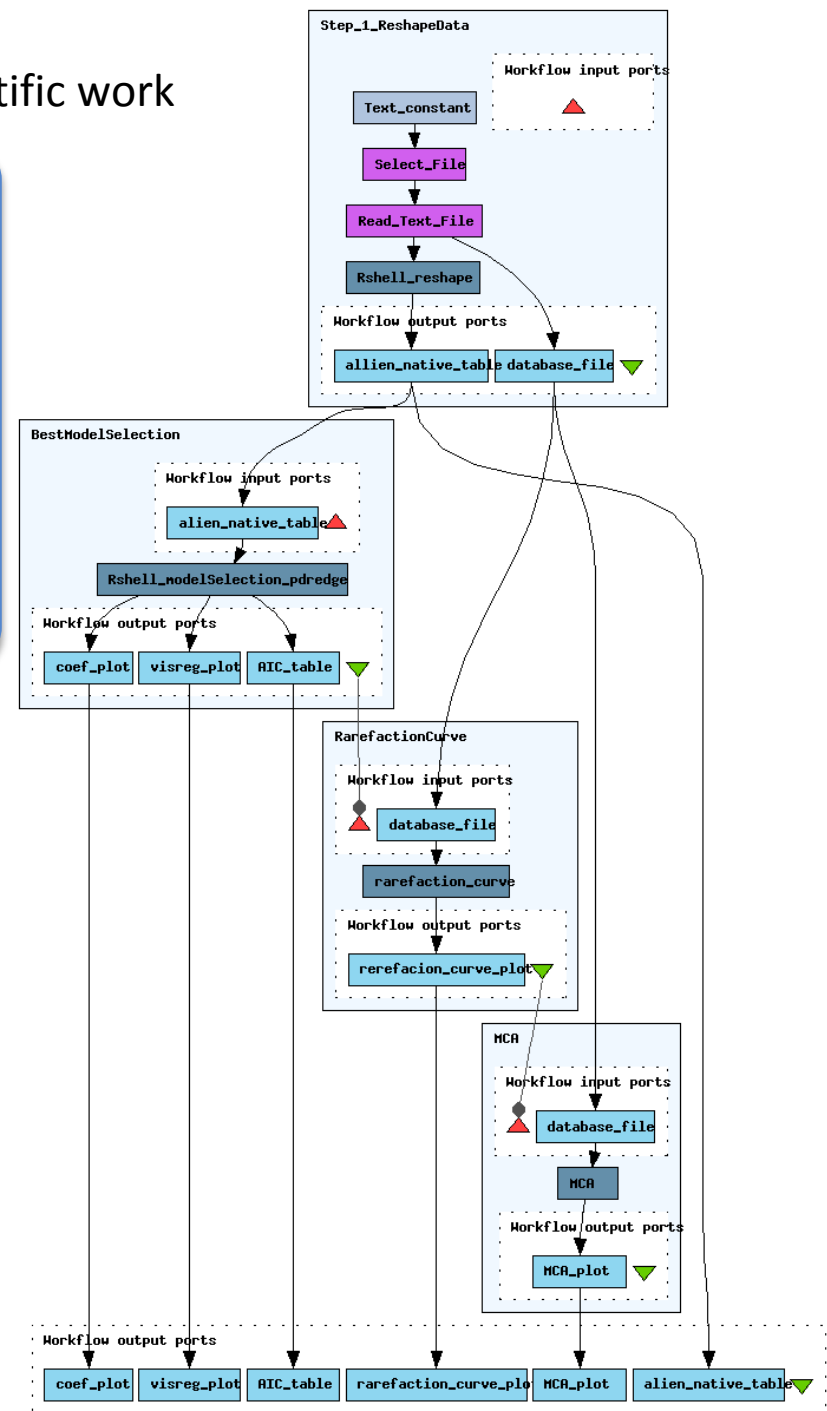
# The workflow as a runnable formalization of scientific work

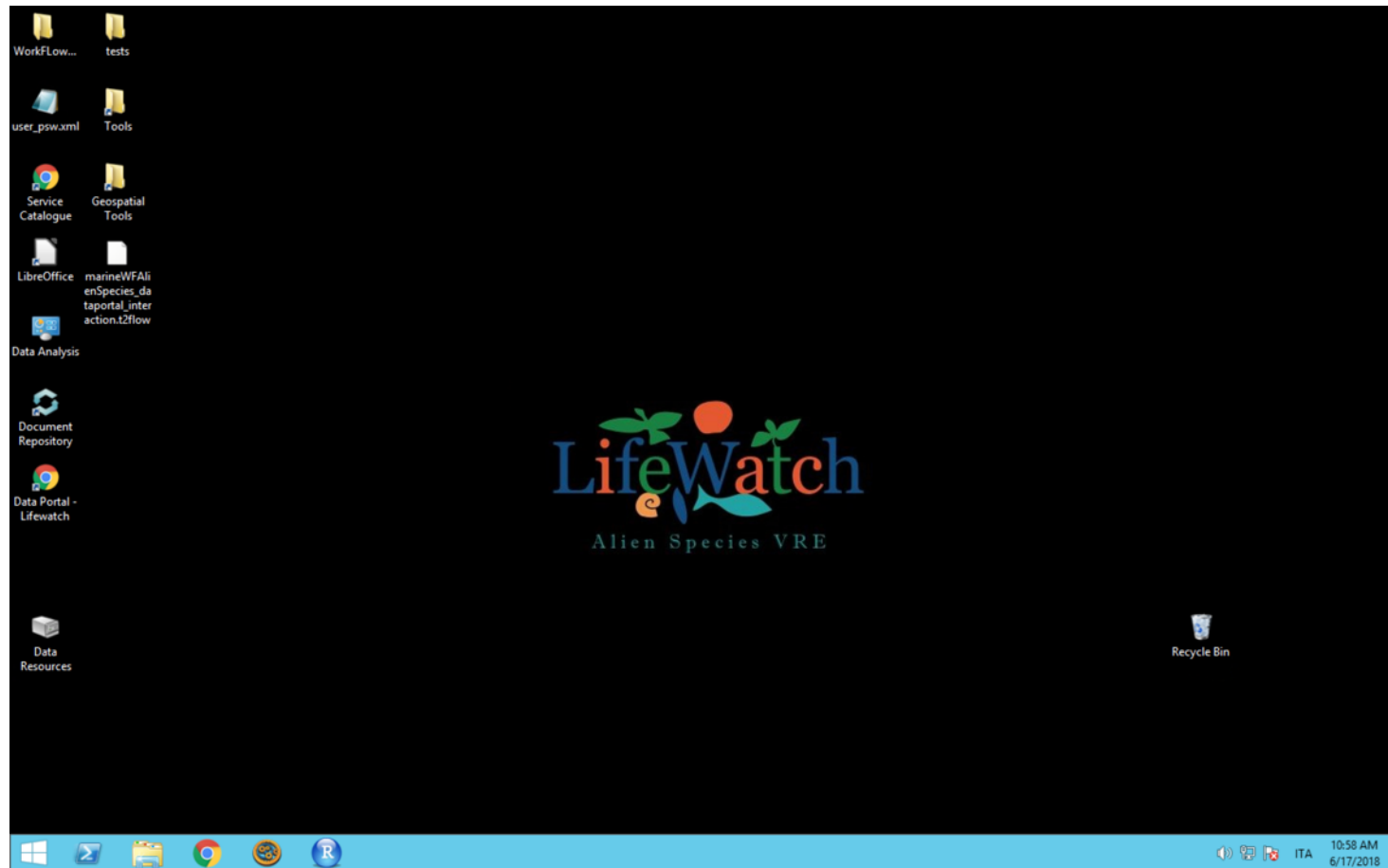
## Taverna workflow system

- Composed by “services” (remote and local) – configurable assignment to agents
- Workflow execution: data driven (plus control links)
- Nested workflows



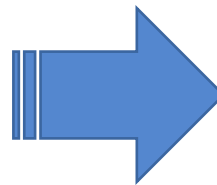
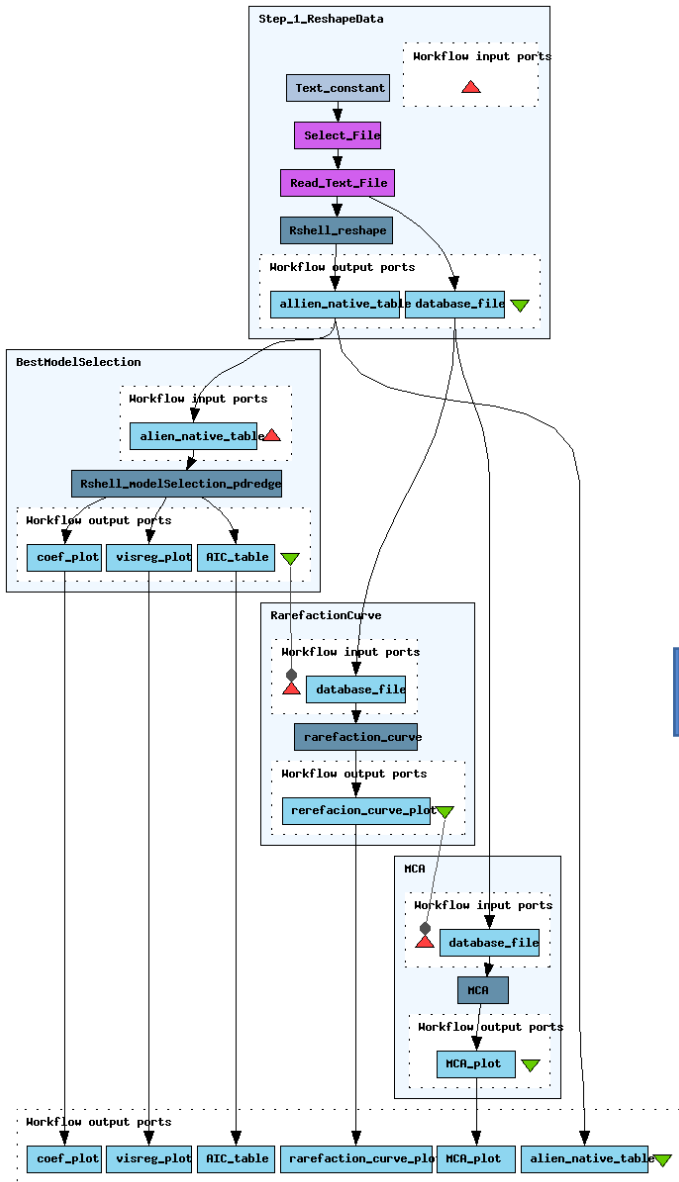
## Example workflow: alien species





- Possibility to replicate the AS showcase analysis
- Possibility to use new data that are stored in the LW dataportal
- Allow some degree of workflow manipulation
  
- Needs to develop new app or web services
- Authentication with multiple users on the same project is triky
- Taverna is not for all

# Complex workflows and researchers...



# What biodiversity researchers want from a VRE?

1. Access to a wide range of biodiversity data (data catalogues)
2. High computing capacity (HPC clusters);
3. Access to a wide range of software validated by the scientific community;
4. A collaborative environment
5. User friendly interface, accessible via web technologies

# Access to biodiversity data

WorldClim - Global Climate Data

*Free climate data for ecological modeling and GIS*







**BEAST**

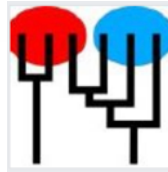
Bayesian evolutionary analysis by sampling trees

**EcoSIM**

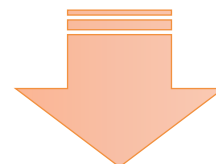
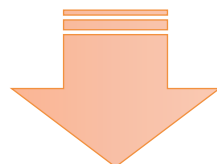
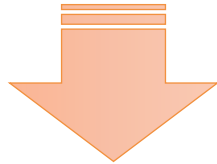


**CIPRES**

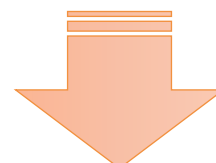
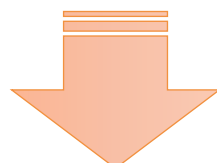
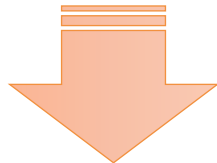
Cyberinfrastructure for  
Phylogenetic Research



Migrate-n

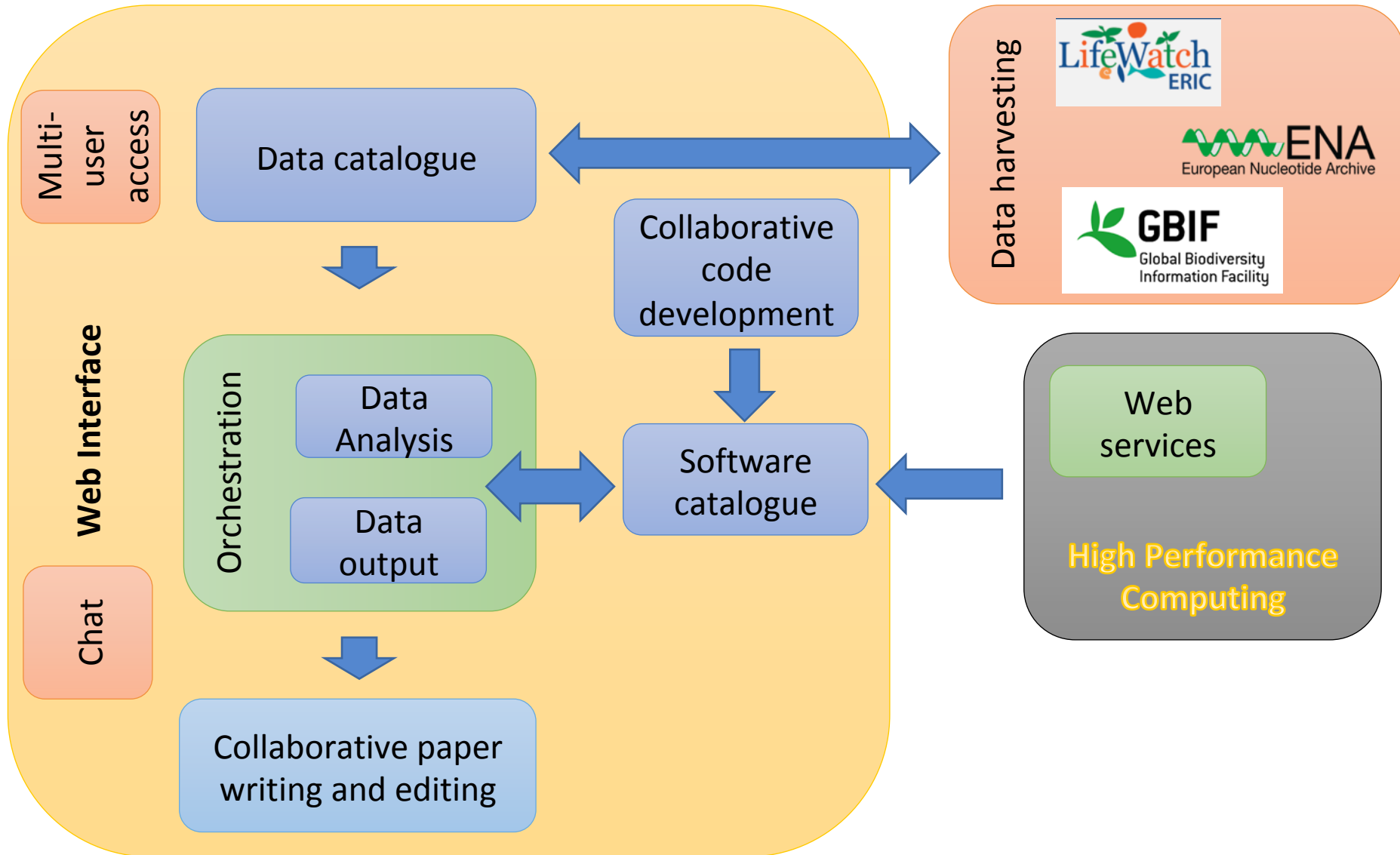


**Web Services catalogue**



**Data analysis**

# VRE-LW architecture



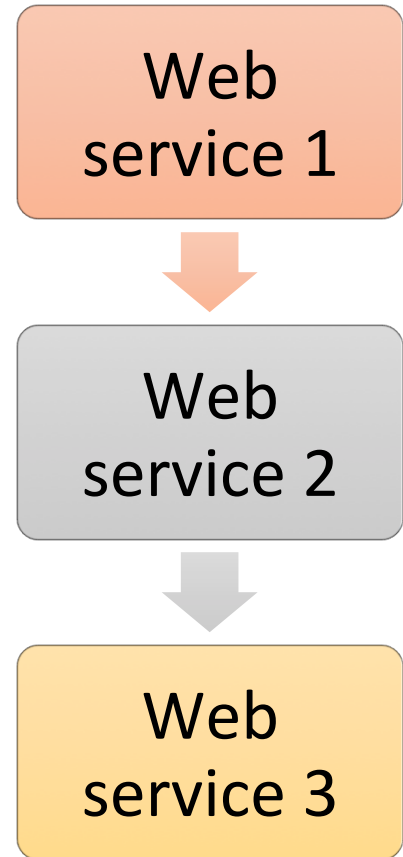
# Orchestrating web services



Taverna



**Different solutions possible, but be aware always to the researchers sensibility...**



# Conclusions

- The access to VREs should lead to faster research results by providing data, tools, computational resources and a collaborative environment
- If the intention is to improve the research process and not simply to show technologies for their own sake, the requirements of users (researchers) must drive the VRE developments

# Conclusions

**If the intention is to improve the research process and not simply to show technologies for their own sake, the requirements of users (researchers) must drive the VRE developments**


**Virtual Research Environments should be designed, since the beginning, to *promote uptake, ensure usability, and guarantee sustainability*. These three aspects form a virtuous circle that, if properly managed, ensure the success of a specific VRE.**

As regards *usability*, **Virtual Research Environments building should be mainly a community building process rather than a technology development process.** This implies that the focus should be primarily on using technology to identify and rationalise workflows, procedures, and processes characterising a certain research scenario rather than having technology invading the research scenario and distracting effort from its real needs.

*Candela et al. (2013). Virtual Research Environments: An Overview and a Research Agenda. Data Science Journal. 12, pp.GRDI75–*

**Statistical workflow**  
Drivers of occurrence/richness  
at site and/or Eunis habitat level

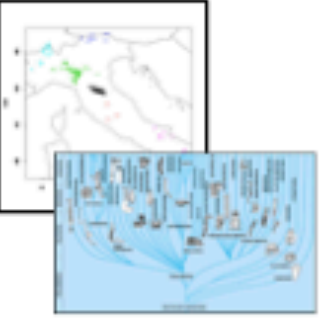
Original database  
Many taxa, habitat, pressures



Variable extraction from  
Geo-referenced rasters  
(pressure, abiotic, biotic)



Structures in the  
dataset



Subsetting, reshaping

Merging

Presence/absence  
matrix

Data matrix for  
modeling  
(Non-normal distributed data)

Ordination  
techniques  
PCA, MCA

Rarefaction  
curves

GLMM  
General linear  
mixed models

Output  
Graphics, tables

Output  
Graphics

Output  
Graphics, tables